Behavior of the Finite-Sized, Three-Dimensional, Ising Model near the Critical Point

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Abstract Recent work showing the validity of hyperscaling involved results for finite size systems very near the critical point. We study this problem in more detail, and give estimators related to the Binder cumulant ratio which seem to approach the critical temperature from above and below. Based on these results, we estimate that the renormalized coupling constant, computed for the temperature fixed at the critical temperature and then taking the large system-size limit, is about 4.9 ± 0.1, and give a likely lower bound for it of 4.5. These estimates are argued to suffice to show the validity of hyperscaling.

The standard, sample problem in the study of critical phenomena is the Ising model. At a critical point in, for example, the temperature – magnetic field plane, many of the thermodynamic properties of a magnet become singular like some, often non-integer, power of a measure of the distance to the critical point in this plane. There are a number of these properties and the exponents describing their singular behavior are called critical indices. One of the long-standing problems in the study of the Ising model has been the validity of hyper-scaling. This property relates to the question of whether the relations between the critical indices which involve the spatial dimension hold or not. One of the key measures of the validity of hyperscaling is whether the quantity,

$$g(K) \equiv - \lim_{L\to\infty} \left(\frac{v}{a^d}\right) \frac{\frac{\partial^2 \chi(K)}{\partial H^2}}{\chi^2(K)\xi^d(K)}, \tag{1}$$

vanishes as the inverse temperature K approaches the critical-point value K_c for the magnetic field H at its critical value of zero. Here d is the spatial dimension, v is the volume of a lattice cell, a is the lattice spacing, L is the system size, χ is the magnetic susceptibility, and ξ is correlation length. If $\lim_{K\to K_c} g(K) \equiv g^* = 0$, then hyperscaling may fail, otherwise it holds.

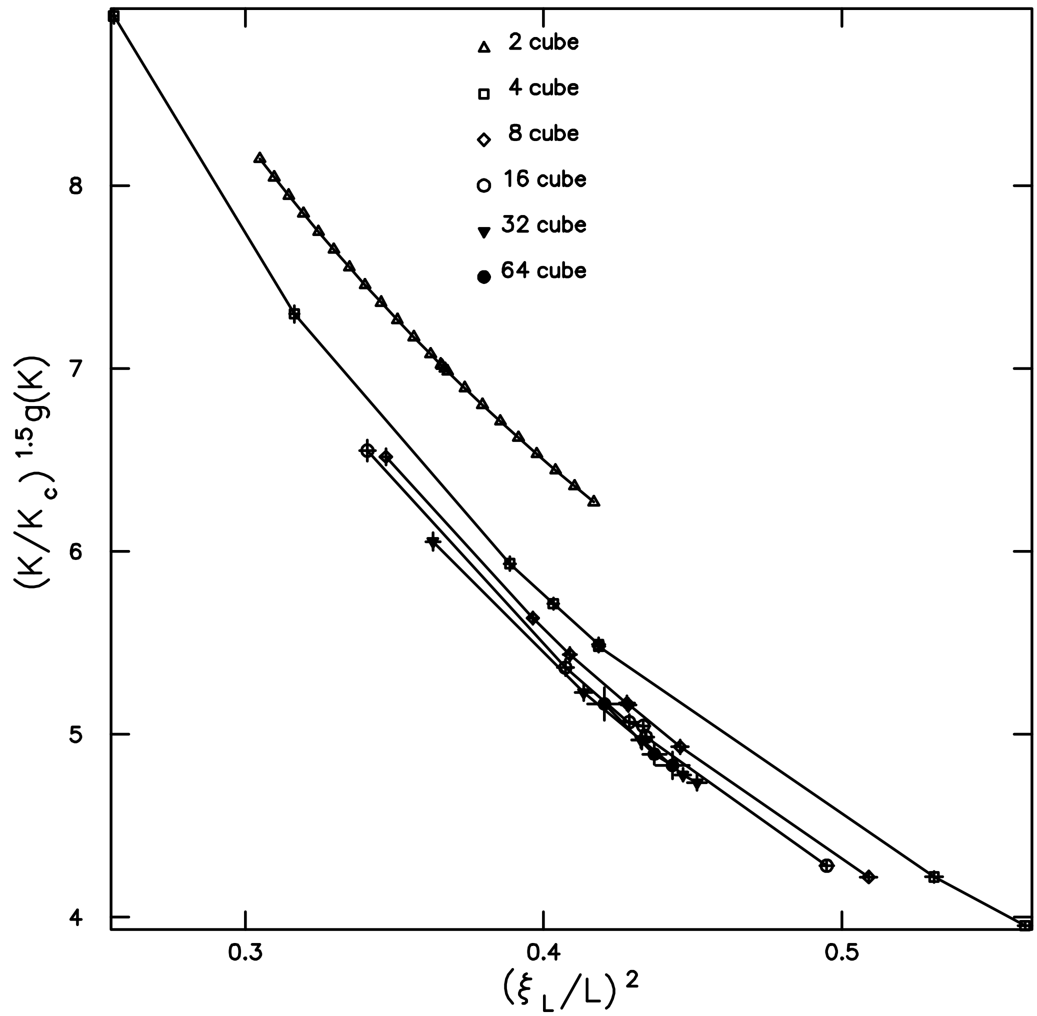

Fig. 1. Monte Carlo results for $g(K,L)(K/K_c)^{1.5}$ *vs.* $(\xi_L/L)^2$ for the three dimensional Ising model.

In his study by exact calculation of the two-dimensional, Ising model, Baker [1] found that the critical point in the temperature – system-size plane is a point of non-uniform approach, *i.e.*,

$$g^* = \lim_{K\to K_c} \lim_{L\to\infty} g(K,L) \neq \lim_{L\to\infty} \lim_{K\to K_c} g(K,L) = \hat{g}. \tag{2}$$

The first of these two limits is the thermodynamically relevant one. Baker and Kawashima [2] recently found that the second of these two limits can be taken as a lower bound on the first, and so the question of whether $g^* > 0$ or not could be answered, if one could show that the second limit $\hat{g} > 0$.

A key feature to notice in analysing the nature of $\hat{g}$ is the observation of Baker and Erpenbeck [3] that, for the three-dimensional, Ising model in the range where ξ_L/L is bounded away from zero, $(K/K_c)^{1.5} g(K,L)$ plotted

Table 1. Table of the curve crossing values of K, g, $(\xi_L/L)^2$ and U.

$n \otimes 2n$	$K_{g,\otimes}$	$g_\otimes$	$K_{\xi,\otimes}$	$(\xi_L/L)^2_\otimes$	$K_{U,\otimes}$	$U_\otimes$
$2 \otimes 4$	0.2135±2	8.24±3	0.2164±2	0.337±1	0.2274±3	–1.5836±7
$4 \otimes 8$	0.2209±1	5.77±6	0.2213±2	0.411±6	0.2227±1	–1.501±4
$8 \otimes 16$	0.22156±7	5.2±1	0.22161±4	0.426±5	0.22201±2	–1.489±2
$16 \otimes 32$	0.22164±2	5.1±1	0.22165±1	0.432±3	0.22168±2	–1.425±9
$32 \otimes 64$	0.22165±1	5.0±2	0.22165±2	0.428±10	0.22166±1	–1.414±7

against ξ_L/L converges fairly rapidly as $L \to \infty$ to a single function. We have done more calculations of these quantities for the three-dimensional, Ising model on the simple-cubic lattice, using the same computer code as in [2] which is a Swendsen-Wang [4] procedure with improved estimators. The results are displayed in Fig. 1. The reason for the factor of $(K/K_c)^{1.5}$ is to keep the quantity plotted finite as $K \to 0$, and unchanged at the critical point. We have used the estimate of Gupta and Tamayo [5], $K_c \approx 0.221655$ here. This value also agrees within error with the recent results of Blöte *et al.* [6], $K_c \approx 0.2216546 \pm 10$.

In the limit as the system size becomes large, the Binder [7] cumulant ratio, $U = \langle M^4\rangle/(\langle M^2\rangle)^2 - 3$, where M is the sum over the lattice of the Ising spins, is zero for $K < K_c$, minus two for $K > K_c$ and some intermediate, fixed-point value U^* for $K = K_c$. Binder has argued that the crossover point of U for successively larger system sizes is a good estimator for the critical temperature. Baker [1] found this proceedure to be about an order of magnitude better than using the peak in the susceptibility. He also noted that the structure of the approach to the infinite, system-size limit is such that the renormalized coupling constant must also display a similar set of crossover points giving estimates of the critical temperature. For the purpose of computing the crossing it is useful to have systematically varying curves, such as used by Gupta and Tamayo [5]. They used a histogram reweighting scheme. To the same end, we have used the same sequence of random numbers for the various different temperatures on the same system size. In addition we have made a series of runs with independent sets of random numbers for the different sized systems at $K = 0.221655 \approx K_c$. The values of the crossings found for K, g, $(\xi_L/L)^2$, and U are listed in Table 1. The 2^3 results were done exactly, numerically. The 4^3, 8^3, and 16^3 were run 300,000 Monte Carlo sweeps or 400,000 for some of the 16^3 cases. The 32^3 and 64^3 were run 400,000 Monte Carlo sweeps, except for U for $L = 64$ the better

Table 2. Table of finite size values
for $K = 0.221655 \approx K_c$.

L	$U(K)$	$(\xi_L/L)^2$	$g(K)$	$g'(K)$	$g(K_{U,\otimes}, L)$
2	–1.55264	0.36584	7.01740	–140	
4	–1.483±2	0.418±2	5.49±4	–390	3.96±11
8	–1.445±2	0.428±2	5.16±4	–780	4.40±11
16	–1.421±3	0.430±2	5.05±3	–1900	4.26±7
32	–1.410±4	0.433±3	4.97±4	–6800	4.8±2
64	–1.407±4	0.437±4	4.89±6	-14000	4.9±2
128	–1.404±4				
256	–1.397±6				

data of Gupta and Tamayo [5] was used. Initialization was several hundred sweeps, with the number increasing with system size. These crossings have been determined by linear interpolation from our data. The quoted errors are single standard deviations and are in units of the last figure quoted. It is to be noticed that, within error, the crossing values for g and $(\xi_L/L)^2$ move to higher values of K, while those for U move to lower values giving confidence that we may have, within our error, bracketed the critical temperature. The results from U are not in contradiction with those of [5], where there is seen some possibility of non-monotonic behavior. The errors prevent us from making a clear distinction here. Thus our results bracket from above and below, within their errors, the value of K_c proposed in refs. [5 & 6]. The results for the crossing values for g are in contrast to the results in two dimensions [1], where the crossing value of K decreases with system size and the value of g at the crossing increases.

The error, $|K_{g,\otimes} - K_c|$, appears to be very roughly proportional to L^{-3} for the crossing values determined by $g(K)$. The rate that $g(K_{g,\otimes})$ approaches $\hat{g}$ is just a reflection in the curve of Fig. 1 of rate of approach of $K_{g,\otimes}$ to K_c. The rates of convergence of the other series are less clear.

We report in Table 2, in analogy with the presentation of ref. [1], the values taken at our estimated critical point as the system size increases. We are able to extend the system-size for U to $L = 128,\ 256$ by the use of the data of ref. [5]. The cross comparison of this data with the current calculations for $L = 64$ is within the error bars. The same extension can not be made for the other quantities as the extrapolation of the estimator of ξ_L to zero momentum was not incorporated in the analysis of [5]. This difference is irrelevant for the thermodynamic limit, g^*, but leads to about a 10% difference in $\hat{g}$. It is to be noted that values of g, $(\xi_L/L)^2$ and U appear to converge rapidly as the system size increases, and the system-size variation disappears into the error near the bottom of the table. The picture of $g(K)$ presented in refs. [1 & 2] envisions a slope which rapidly increases with system size at the critical point to accommodate $g^* \neq \hat{g}$. This view is well supported by the (very rough) values of $g'(K)$ which were obtained by numerical differentiation and are displayed in Table 2. These values increase roughly proportional to $L^{4/3}$. A more detailed study of the slopes of other quantities was given in ref. [5].

In the last column of Table 2, we give the values of $g(K,L)$ at the crossing point of $U(K,L)$ and $U(K,\frac{1}{2}L)$. As remarked above, this crossing point seems to be an upper bound for K_c. As g is a decreasing function of K, this quantity should be a lower bound for $\hat{g}$. We note that $g(K_{U,\otimes},L)$ as just defined and tabulated in Table 2, is a generally increasing function of the system size, L. There is a competition reflected here between the increase in the slope of g and shown in the previous column which tends to lower the value, and the rate of convergence of $K_{U,\otimes}$ which tends to increase the value. As the latter seems to be dominate, asmptotically, we have thus constructed what appears to be numerically, an asymptotically increasing lower bound to $\hat{g}$. Hence, from the values in Table 2, we conclude at the 2 standard error level that $g^* > \hat{g} \gtrsim 4.5 > 0$. This more through study bolsters the conclusion of ref. [2], that $g^* > 0$ and so that hyperscaling holds. Note that the same type arguments applied to the results in Table 1, indicate further likely bounds. If we use two standard errors then we find $5.4 \gtrsim \hat{g}$. Similarly we find a lower bound for the large system limit of $(\xi_L/L)^2$ of 0.426, and $U^* \gtrsim -1.43$.

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